

A dilute mixture of atoms and molecules

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Abstract

We study a dilute gas with two species of Fermionic atoms of unequal concentrations, interacting via a short-range interaction with one deeply bound state. We study the properties of this system under the mean-field approximation. We obtain the effective interaction among the fermions and bosons, and discuss the collective modes of the system.

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Recent experimental advances in trapping and cooling alkali atoms have already given us condensates of Bosons [1] and degenerate gases of Fermions [2,3]. Much theoretical and experimental efforts have now turned to systems with trapped molecules, with interesting observations and predictions on the equilibrium and dynamical properties of this system. [4–9] These molecules can have their constituent atoms be either Bosons or Fermions. [10] The latter case, on which the rest of this paper will concentrate, is also of particularly interest when it is considered together with superfluidity arising from Cooper pairing of Fermions. Indeed superfluid ^3He and most known superconductors have their superfluidity derived from Cooper pairs. It is also widely believed that Fermionic pairing in diatomic molecules and in Cooper pairs are in fact two limits of a continuum. [11] Much work has already been devoted to the cross-over between these two limits. [12,13] (and references therein) There is also a lot of interest in producing pairs (within any part of the above mentioned continuum) in trapped atomic Fermions. [10]

We here would like to further our understanding of systems consisting of "molecules". We shall limit ourselves to "molecules" made up of two distinguishable Fermions, interacting

via a short range ($\ll a$ below) interaction, in the s-wave state (Therefore by 'molecule' we simply mean the Boson made up by a pair of Fermions). These two partners of the molecule can in general be atoms in different hyperfine spin projections or internal states, or different atomic species. For definiteness we shall restrict ourselves to the first case and for simplicity refer them hereafter as spin "up" and "down", with concentrations n_\uparrow and n_\downarrow . We shall study the properties of this system when the two constituents of the molecule are of different concentrations, say when $n_\uparrow > n_\downarrow$. Furthermore, we restrict ourselves to the case where the size of the bound state a is small, such that $n_\uparrow a^3$ and $n_\downarrow a^3$ are both much smaller than 1. Then at temperatures much below the dissociation temperature T_{disso} all down spins are paired into molecules but there are left over (or excess) spin-up Fermions. The Bosonic molecules and Fermionic atoms basically do not overlap and are well-defined entities. Thus one has a Bose-Fermi mixture where the Fermions are identical with one of the constituent particles of the Bosons, with the Boson and Fermion concentrations $n_b = n_\downarrow$ and $\nu = n_\uparrow - n_\downarrow$ respectively.

We shall obtain the properties of our Bose-Fermi mixture by applying many-body techniques on the (more basic) constituent spin-up and down Fermions (generalizing ref [11–13] — we shall also be following the notations of the last reference quite closely, except that we shall use the more common sign conventions for the single particle propagators and self-energies). This system is attractive theoretically in that all interactions can be characterized by one interaction parameter, namely the s-wave scattering length a (> 0) between the spin up and down Fermions, or equivalently the binding energy ϵ_b of the molecule ($\epsilon_b = \hbar^2/ma^2$, here m is the mass of either of the Fermions). There are, however, several energy scales and hence temperature regimes. As mentioned we shall limit ourselves to where the temperature T of the system is much lower than the dissociation temperature T_{disso} ($\sim \epsilon_b$ up to some entropic factors). The relevant scales are thus T , the Bose-Einstein condensation temperature T_{BEC} for the Bosons and the Fermi temperature T_F for the (left-over) Fermions ($T_{\text{BEC}} \sim n_b^{2/3} \hbar^2/m$ and $T_F \sim \nu^{2/3} \hbar^2/m$. Note they are much less than T_{disso}). We shall study the some properties of this system at $T = 0$ and compare them with those of a general

dilute Bose-Fermi mixture. In particular, we shall be able to find the effective interaction, or equivalently the scattering length, between the Bosons and Fermions in terms of a . We further show that the Bogoliubov mode of the system is the same as that of a Bose-Fermi mixture.

In the case where the pairing between the spin-up and down particles are in the Cooper limit (weak attractive interaction so that $a < 0$ and small), the system with $n_\uparrow > n_\downarrow$ has been studied before in the context of superconductivity under an applied Zeeman field h [14]. We shall compare our results with those of this better known system.

We now consider the system at $T = 0$ under the mean-field approximation. The necessary mean field equations can be obtained by generalizing those of ref [11] (which deals with $n_\uparrow = n_\downarrow$). We introduce three fields, the chemical potentials $\mu_\uparrow, \mu_\downarrow$ for the two spin species and a pairing field Δ . These fields obey the self-consistent equations

$$1 = \frac{4\pi\hbar^2 a}{m} \int_{\vec{k}} \left[\frac{1}{2\epsilon_k} - \frac{1}{2E_k} (1 - f(E_k - h) - f(E_k + h)) \right] \quad (1)$$

$$n_\sigma = \int_{\vec{k}} n_\sigma(\vec{k}) \quad , \quad \sigma = \uparrow \text{ or } \downarrow \quad (2)$$

with

$$n_\uparrow(\vec{k}) = u_k^2 f(E_k - h) + v_k^2 (1 - f(E_k + h)) \quad (3)$$

$$n_\downarrow(\vec{k}) = u_k^2 f(E_k + h) + v_k^2 (1 - f(E_k - h)) \quad (4)$$

where f is the Fermi function. We have defined for convenience the chemical potential average and difference $\mu \equiv (\mu_\uparrow + \mu_\downarrow)/2$, $h \equiv (\mu_\uparrow - \mu_\downarrow)/2$ (> 0), the energies $\epsilon_k \equiv \hbar^2 k^2/2m$, $E_k \equiv [(\epsilon_k - \mu)^2 + |\Delta|^2]^{1/2}$, and the "coherence factors" $u_k^2 = \frac{1}{2}(1 + \frac{\epsilon_k - \mu}{E_k})$, $v_k^2 = \frac{1}{2}(1 - \frac{\epsilon_k - \mu}{E_k})$, $u_k v_k = \frac{\Delta}{2E_k}$ are exactly as in BCS theory for superconductivity. Eq (1) is the self-consistent equation for Δ whereas eqs (2) are the constraints for the Fermion concentrations, with $n_\sigma(\vec{k})$ the occupation number at wavevector \vec{k} . Notice that if we view the system as a Bose-Fermi mixture, the chemical potential for the Bosons is $\mu_b = 2\mu$ and that for the (left-over)

Fermions is μ_\uparrow . In the dilute limit $0 < x_\uparrow \equiv n_\uparrow a^3 \ll 1$ and $0 < x_\downarrow \equiv n_\downarrow a^3 \ll 1$ which we are studying (in contrast to the Cooper limit where $a < 0$), it is convenient to study the solution to eqs (1)-(2) as an expansion in x_\uparrow and x_\downarrow . At $T = 0$, $f(E_k + h) = 0$ and $f(E_k - h)$ is non-vanishing only for $k < k_c$ where $E_{k_c} = h$. From eq (3) and (4) we get immediately

$$\nu = k_c^3/6\pi^2. \quad (5)$$

k_c plays the role of the Fermi wavevector for the excess spin-up Fermions (which form a ‘Fermi sea’, see also below)

We shall see (as in the corresponding case of ref [11]) that $\mu < 0$ and $|\Delta| \ll |\mu|$. Using this inequality, eq(1) and eq(4), we obtain two equations determinating Δ and μ . In the dilute limit we get

$$\mu = -\frac{\hbar^2}{2ma^2} + \frac{2\pi(n_b + 2\nu)\hbar^2 a}{m} \quad (6)$$

$$|\Delta|^2 = 8\pi n_b \epsilon_b^2 a^3 [1 - \dots] \quad (7)$$

(and hence $|\Delta|^2/\mu^2 \sim n_b a^3 \ll 1$ as promised). Eq (6) can be interpreted easily by recalling $\mu_b = 2\mu$. The first term arises from the binding energy of the molecule. The two parts of the second term represent the mean-field corrections to the chemical potential due to the interaction of the molecules among themselves and with the Fermions respectively. Equating these two expressions with (1/2 times) $n_b g_{bb}$ and νg_{bf} , we obtain the interaction constants

$$g_{bb} = \frac{4\pi\hbar^2 a}{m} \quad (8)$$

$$g_{bf} = \frac{8\pi\hbar^2 a}{m} \quad (9)$$

or equivalently the scattering lengths $a_{bb} = 2a$ and $a_{bf} = 8a/3$. [15]

We now discuss some properties associated with the Fermions. The occupation numbers of the constituent Fermions $n_\sigma(\vec{k})$ are sketched in Fig. 1 for $T = 0$. $n_\uparrow(k) = 1$ whereas $n_\downarrow(k) = 0$ for $k < k_c$. $n_\uparrow(k)$ and $n_\downarrow(k)$ are equal but small for $k > k_c$. These results can be understood by considering the wavefunction of the system [16].

It is also interesting to study the spectral function $A_{\uparrow}(\vec{k}, \omega)$ ($= -\frac{1}{\pi} \text{Im } G_{\uparrow 11}^R(\vec{k}, \omega)$ given below) corresponding to the density of states for addition/removal of a spin-up Fermion at momentum \vec{k} and energy ω . $A_{\uparrow}(\vec{k}, \omega)$ has the same formal expression as in the case of Cooper pairing (c.f. eq (12) below): $A(\vec{k}, \omega) = u_k^2 \delta(\omega - (E_k - h)) + v_k^2 \delta(\omega + (E_k + h))$. There are thus two delta-function peaks, one at positive and one at negative energies. Since $|\Delta| \ll \mu$, $v_k^2 \ll 1$ and thus the weight at the negative frequency is very small. To a very good approximation, $A_{\uparrow} \sim \delta(\omega - (\epsilon_k - \mu_{\uparrow}))$, that of a free Fermi gas. We shall compare these results with those of case (B) below.

We next study the dynamic properties of our system (at $T = 0$) by evaluating the two particle vertex function (matrix) $\mathbf{\Gamma}(Q, \Omega)$ for repeated scattering between a spin-up and spin-down particle (hole) at small wavevector Q and frequency Ω . We shall see that, as in the case of $n_{\uparrow} = n_{\downarrow}$, [12,13] $\mathbf{\Gamma}$ is related to the propagator for the Bosons. $\mathbf{\Gamma}$, in Matsubara frequencies (we shall drop the superscript M for simplicity. The desired $\mathbf{\Gamma}$ in real frequency can be obtained via $i\Omega_{\nu} \rightarrow \Omega$ with $\Omega_{\nu} > 0$ as usual) obeys the Bethe-Salpeter equation (generalizing that of [13])

$$\Gamma_{\alpha 1, \alpha 2}^{-1}(Q, \Omega_{\nu}) = \frac{m}{4\pi\hbar^2 a} \delta_{\alpha 1, \alpha 2} + M_{\alpha 1, \alpha 2}(Q, \Omega_{\nu}) \quad (10)$$

where

$$M_{\alpha 1, \alpha 2}(Q, \Omega_{\nu}) \equiv \int_{\vec{k}} \left[T \sum_{\epsilon_n} G_{\uparrow \alpha 1, \alpha 2}(\vec{Q} - \vec{k}, \Omega_{\nu} - \epsilon_n) G_{\downarrow \alpha 1, \alpha 2}(\vec{k}, \epsilon_n) - \frac{m}{\hbar^2 k^2} \delta_{\alpha 1, \alpha 2} \right] \quad (11)$$

and $G_{\sigma \alpha 1, \alpha 2}$ are the matrix Green's function in particle ($\alpha = 1$) and hole ($\alpha = 2$) space for spin- σ defined in a similar manner as in Gorkov's theory of superconductivity [17], and Ω_{ν} and ϵ_n are Bosonic and Fermionic Matsubara frequencies respectively. In principle there is a contribution to the self-energy for \mathbf{G} proportional to $\mathbf{\Gamma}$ and therefore \mathbf{G} and $\mathbf{\Gamma}$ have to be found self-consistently (see [13]). However, at $T = 0$ and under our diluteness condition we can simply use the mean-field solution for G , *i.e.*,

$$G_{\uparrow 11}(\vec{k}, \epsilon_n) = \frac{u_k^2}{i\epsilon_n - (E_k - h)} + \frac{v_k^2}{i\epsilon_n + (E_k + h)} \quad (12)$$

and

$$G_{\uparrow 12}(\vec{k}, \epsilon_n) = u_k v_k \left[\frac{1}{i\epsilon_n - (E_k - h)} - \frac{1}{i\epsilon_n + (E_k + h)} \right] \quad (13)$$

where u_k, v_k are the coherence factors introduced before. G_{\downarrow} 's are given by similar expressions except $h \rightarrow -h$ and $\Delta \rightarrow -\Delta$. $\Gamma^{-1}(Q = 0, \Omega_\nu = 0)$ can be calculated easily and is of order Δ^2 due to eq (1). However, evaluation of Γ^{-1} at finite Q and Ω needs special care. In M_{11} there arises the contribution

$$\begin{aligned} M_{11}^a(Q, \Omega) &\equiv - \int_{\vec{k}} u_{\vec{Q}-\vec{k}}^2 v_{\vec{k}}^2 T \sum_{\epsilon_n} \left[\frac{1}{i\epsilon_n + (E_{\vec{Q}-\vec{k}} - h) - \Omega} \times \frac{1}{i\epsilon_n + (E_{\vec{k}} - h)} \right] \\ &= \int_{\vec{k}} u_{\vec{Q}-\vec{k}}^2 v_{\vec{k}}^2 \frac{[1 - \text{sgn}((E_{\vec{Q}-\vec{k}} - h) - \Omega) \text{sgn}(E_{\vec{k}} - h)]/2}{|E_{\vec{Q}-\vec{k}} - E_{\vec{k}} - \Omega|} . \end{aligned}$$

The integrand is singular as Q and Ω approaches 0. To evaluate M_{11}^a , we first note that under our diluteness approximation, we can replace E_k by $\epsilon_k - \mu$ and thus $E_k - h = E_k - E_{k_c} \approx \epsilon_k - \epsilon_{k_c}$ etc. The integrand is therefore finite only if $\epsilon_{\vec{Q}-\vec{k}_c} - \epsilon_{k_c} - \Omega$ and $\epsilon_k - \epsilon_{k_c}$ are of opposite signs, and thus for $Q \ll k_c$, $\Omega \ll k_c^2/m$, \vec{k} is restricted to be near the "Fermi surface", i.e., $|\vec{k}| \sim k_c$. We can then use $u_{\vec{Q}-\vec{k}}^2 v_{\vec{k}}^2 \approx u_{k_c}^2 v_{k_c}^2 \approx \left(\frac{|\Delta|}{\epsilon_b}\right)^2$, and replace the \vec{k} integral by integration over \hat{k} and $\xi_k \equiv \epsilon_k - \epsilon_{k_c}$. We finally obtain $M_{11}^a(Q, \Omega) \approx \frac{mk_c}{2\pi^2} \left(\frac{|\Delta|}{\epsilon_b}\right)^2$, and hence

$$-\Gamma_{11}^{-1}(Q, \Omega) = \frac{1}{8\pi\epsilon_b^2 a^3} \left\{ -\Omega + \frac{Q^2}{4m} + \frac{|\Delta|^2}{2\epsilon_b} - 8\pi|\Delta|^2 a^3 \left(\frac{mk_c}{2\pi^2} \right) \right\} . \quad (14)$$

Similarly

$$-\Gamma_{12}^{-1}(Q, \Omega) = \frac{1}{8\pi\epsilon_b^2 a^3} \left\{ \frac{\Delta^2}{2\epsilon_b} - 8\pi\Delta^2 a^3 \left(\frac{mk_c}{2\pi^2} \right) \right\} . \quad (15)$$

As in the case of equal number of spin-up and down particles, [13] Γ is thus found to be proportional to the connected part of the Bosonic propagator matrix \mathbf{G}_b . \mathbf{G}_b^{-1} , under the random phase approximation, reads (c.f. [18])

$$-G_{b11}^{-1}(Q, \Omega) = -\Omega + \frac{Q^2}{2m_b} + g_{bb}n_b - g_{bf}^2 n_b \chi_f(Q, \Omega) \quad (16)$$

$$-G_{b12}^{-1}(Q, \Omega) = +g_{bb}n_b - g_{bf}^2 n_b \chi_f(Q, \Omega) \quad (17)$$

where χ_f is the density response of the Fermions and we have taken the gauge where the phase of the condensate is zero. To further check our claim that $\mathbf{\Gamma} \propto \mathbf{G}_b$ above, we note that $m_b = 2m$, $g_{bb}n_b = \frac{|\Delta|^2}{2\epsilon_b}$, $g_{bf}^2 n_b = 8\pi|\Delta|^2 a^3$ (using eqs (7), (8) and (9)), $\chi_f(Q, \Omega) = \left(\frac{mk_c}{2\pi^2}\right)$. In this last expression, we have used the value of $\chi_f(Q, \Omega)$ for $\Omega/Q \rightarrow 0$. That this is the correct limit can be seen as follows. The bare sound velocity for the Bosons is given by $c_b^0 = (n_b g_{bb}/m_b)^{1/2}$ whereas the bare Fermi velocity is $v_f^0 = k_c/m$. Thus $(c_b^0/v_f^0)^2 \sim (n_b a/k_c^2) \ll 1$ under our diluteness condition. For the mode under consideration, $(\Omega/v_f Q) \sim (c_b^0/v_f^0) \ll 1$.

In conclusion, we have studied, via many-body technique, some properties of an atom-molecule mixture where the Fermionic atoms are identical with one of the constituent atoms of the diatomic molecules. If $T \ll T_{BEC}$, our system behaves like a general Bose-Fermi mixture. In this case we have also obtained the scattering lengths a_{bb} and a_{bf} for our mixture in terms of a .

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- [15] Eq (8) has been obtained already in [12] by considering $\mathbf{\Gamma}$ for a system with $n_{\uparrow} = n_{\downarrow} = n_b$. One can get both eqs (8) and (9) using reasoning similar to that in text by evaluating instead μ and E_k of this system. From μ one obtains eq (8) as in text. For E_k , one gets

$2E_{k=0} = 2|\mu| + |\Delta|^2/|\mu|$. However, this must equal $|\mu_b| + 2n_b g_{bf}$ by physical arguments. Equating the two expressions one gets again eq (9).

- [16] The (unrenormalized) wavefunction for our system can be written as (generalizing [11]) $\left(\prod_{\vec{k}', k' < k_c} c_{\vec{k}'\uparrow}^\dagger\right) \times \left(\sum_{\vec{k}} \chi(k) c_{\vec{k}\uparrow}^\dagger c_{-\vec{k}\downarrow}^\dagger\right)^{N_b} |\text{vac} \rangle$. Here $c_{\vec{k}\sigma}^\dagger$ is the creation operator of a Fermion with wavevector \vec{k} and spin σ , $\chi(k) = u_k v_k$ the (Fourier transformed) spatial part of the molecular wavefunction, and N_b the total number of Bosons.

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FIGURES

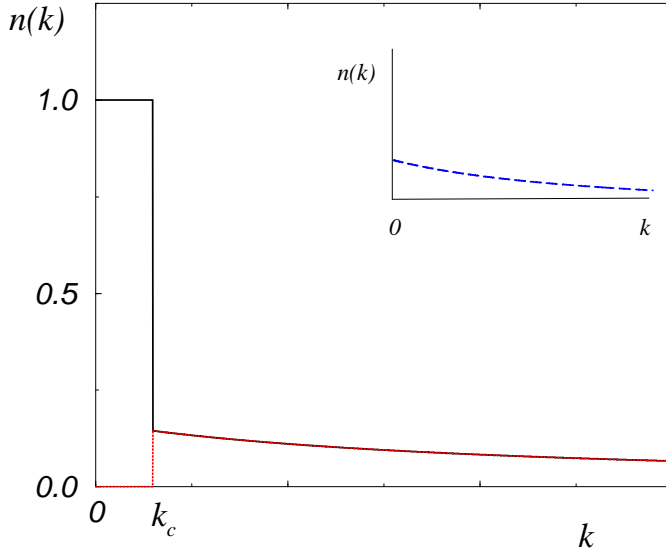


FIG. 1. Schematic plot of $n_{\sigma}(\vec{k})$ versus k . Full line: $n_{\uparrow}(\vec{k})$, dotted line: $n_{\downarrow}(\vec{k})$. The magnitude of $n_{\sigma}(\vec{k})$ for $k > k_c$ has been exaggerated for clarity. Inset: Sketch of $n(\vec{k})$ for the case of $n_{\uparrow} = n_{\downarrow}$.